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DEPC-MPE 034**

**Finite element analysis of the
stress and strain associated
with a corrosion pit in a
cylindrical specimen under
applied tensile loading**

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Finite element analysis of the stress and strain associated
with a corrosion pit in a cylindrical specimen
under applied tensile loading

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ABSTRACT

A finite element analysis has been undertaken to evaluate the stress and strain distribution associated with a single corrosion pit in a cylindrical specimen stressed remotely in tension. Hemispherical and bullet-shaped pits were investigated at stresses corresponding to 90% of the 0.2 % proof stress for a steam turbine disc steel, the pit shapes reflecting, crudely, shallow and deep pits respectively. The key observation was the localisation of plastic strain to the pit walls, just below the surface of the specimen. This localisation of plastic strain correlated with recent X-ray tomography measurements suggesting that stress corrosion cracking was initiated predominantly at or just below the surface, though other factors such as the local electrode potential and chemistry could also be contributing.

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Approved on behalf of the Managing Director, NPL,
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1. INTRODUCTION

Stress corrosion cracks in steam turbine disc steels exposed to simulated condensate tend to emanate from corrosion pit precursors, certainly for the low to medium strength steels¹. However, the evolution of these cracks is not straightforward. Using a layer removal technique involving photographing the specimen surface after every 40 μm of material removed and applying appropriate software a 3-D image of the pit and crack profiles emerged². This image highlighted novel and unusual features such as finger-like cracks emerging from the pits. The other feature was the observation³ of pits whose depth was greater than the associated cracks, with the proportion increasing with shorter exposure times as shown schematically in Figure 1.

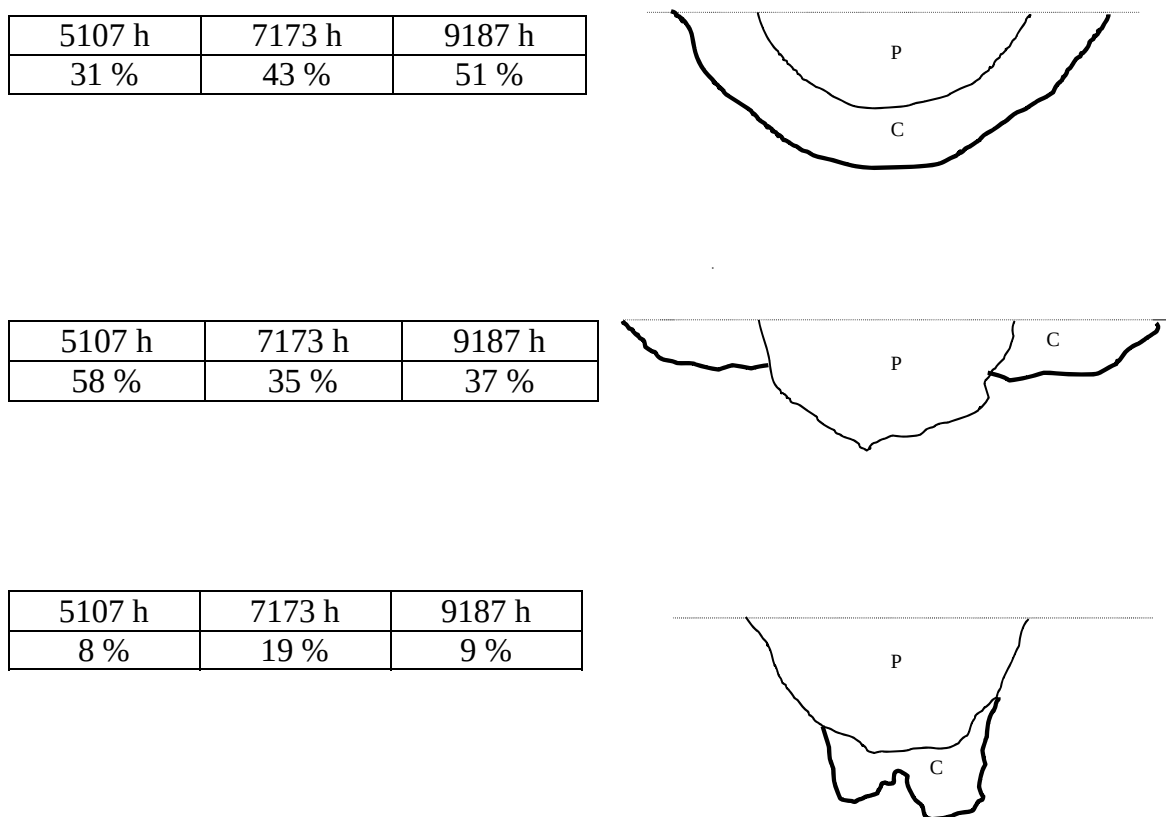
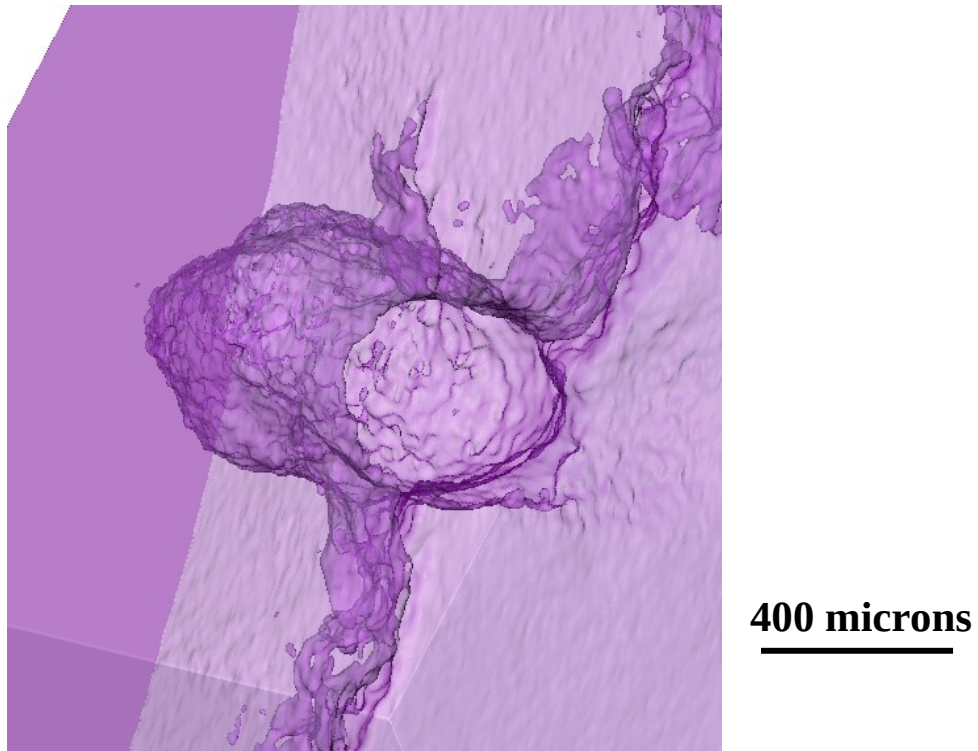


Figure 1. Typical pit and crack profiles in a 3NiCrMoV disc steel exposed at 90° in 1.5 ppm Cl^- at different exposure times showing percentage of different types of profile.

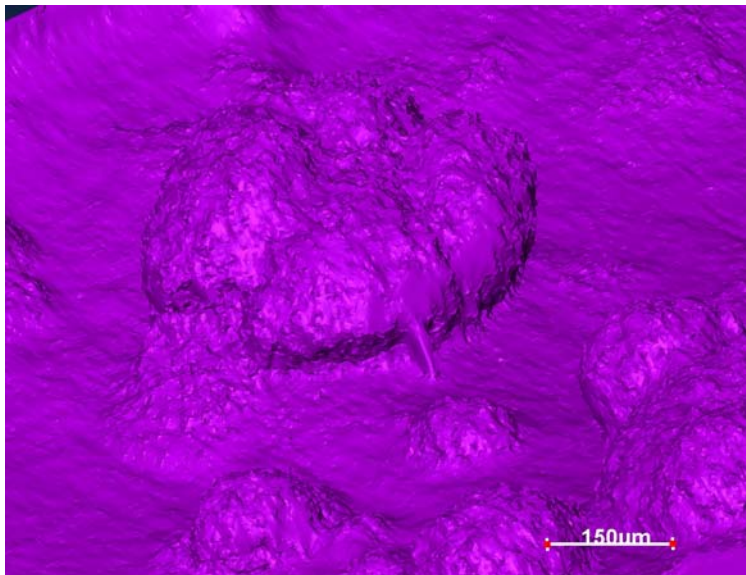
There has to be care in interpreting snapshots at different exposure times but the implication was that in many cases cracks were originating not from the base of the pit but from somewhere on the sides of the pit near the mouth. Conceivably, the cracks could start from the base of the pit and grow to the surface and the pit then outgrows the crack but the consistent observation of a high percentage of cracks emanating close to the open surface of the pits at short exposure times is convincing. Recent X-ray

tomography examination⁴ of specimens removed from solution at shorter exposure times, in the range 168 h to 2160 h, appeared to confirm this. A further observation was that the very deep pits (typically $\geq 600 \mu\text{m}$) tended almost invariably to have cracks of shallower depth. For the same exposure time, the deep pits will be the faster growing pits and the transition to a crack will tend to be restrained until the pit growth rate (which decreases with depth) is sufficiently slow to enable an incipient crack to outrun it.

There are a number of factors that could explain the position sensitivity of crack nucleation, including electrochemical and local topographical features in the pit, but foremost in any assessment should be an evaluation of the stress and strain associated with a corrosion pit. To that aim, a finite element analysis was undertaken for a cylindrical specimen, stressed remotely in tension, containing a single corrosion pit. The aspect ratio of pits in this test system increases with pit depth and exposure time. Nevertheless, for simplicity two geometries were considered: hemispherical and “bullet” shaped (a U-shape in cross section). The latter is somewhat more reflective of the shape of the deeper pits as exemplified by the X-ray tomographic image⁴ of Figure 2a. Hemispherical pits are a crude approximation to shallow pits, an image of which is shown in Figure 2b, with a small crack emerging from the pit wall.



(A)



(B)

Figure 2. X-ray tomographic images of corrosion pit in a disc steel exposed to 1.5 ppm chloride showing (a) almost bullet-like shape for a deep pit with cracks appearing to emanate from the pit walls and (b) surface of shallower pit viewed from underneath showing emerging single crack⁴.

2. DETAILS OF MODEL

Material properties and stress conditions

The mechanical properties appropriate to this analysis for a 3NiCrMoV disc steel are given in Table 1. The test temperature reflects the temperature of the early condensate on a low pressure steam turbine.

Table 1 Mechanical properties (mean values) of the disc steel

Condition	T (°C)	E (GPa)	$\sigma_{0.2}$ (MPa)	UTS (MPa)	Elongation (%)
Stress relieved	90	210	705	827	20

Poisson's ratio for the steel was not measured and a value of 0.3 was adopted.

The analysis makes use of the full stress-strain behaviour of the material and a plot of the data is shown in Figure 3.

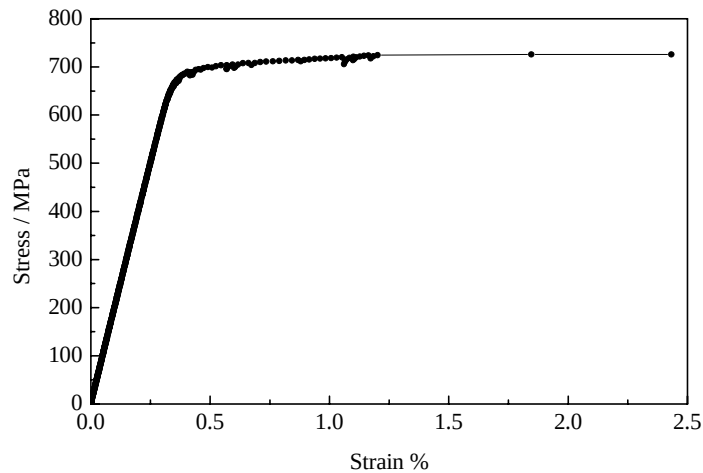


Figure 3. Stress strain behaviour for a 3NiCrMoV steel in air at 90 °C

All computations were made with an applied stress of 90 % of $\sigma_{0.2}$.

3. BASIS OF FINITE ELEMENT ANALYSIS

The FE analysis has been carried out using ABAQUS V6.5-7. A 3-D version of the cylindrical specimen was modelled in the ABAQUS CAE pre-processor. A pit was created half way along the length of the specimen. The pit dimensions could be modified easily in ABAQUS/CAE to investigate the pit size effects. SI (mm) units were used throughout (mm, N, tonne (1E3kg), s, MPa, mJ, tonne/mm³).

The mesh was created using the 3-D elements C3D4, which are 4-node linear tetrahedral elements. The mesh was refined in the region around the pit to enhance the accuracy of stress and strain predictions. When the pit dimensions were changed, the

mesh density around the pit was altered to ensure consistency in the size of the elements created around each pit. This means that the meshes created on the different pits will not be identical but should give similar levels of predictive accuracy. To verify the choice of linear elements, a single analysis was run of the 6.4 mm specimen with 100 μm pit using second order tetrahedral elements (C3D10). Second order elements can be more accurate in certain situations due to the higher number of nodes and integration points in each element. Due to the requirement for the same mesh density around the pit, using these element types greatly increased the size of the model (increased numbers of both nodes and elements). This increased the disk space needed to run the analysis and the run time of the analysis. To obtain an analysis that would run using these second order elements, the mesh needed to be coarser in the bulk of the specimen. Predictions of stress and strain distributions and maximum values were very similar for both element types. Due to these disk space and run time considerations, the linear tetrahedral elements were used.

Boundary conditions were applied to the ends of the specimen to ensure specimen alignment during loading. A uniform stress was applied to the surface at one end of the specimen. The von Mises material model was used in the analysis to characterise the elastic-plastic behaviour of the material.

4. SPECIMEN GEOMETRY

The specimen and pit geometry are illustrated in Figures 4 and 5. The specimen diameter was 6.4 mm to correspond with the stress corrosion tests specimens. However, the effect of increasing the specimen diameter to 32 mm was evaluated also to ensure that deductions from the small diameter specimen had general applicability. For the 500 μm deep bullet-shaped pit the mouth opening was 666 μm .

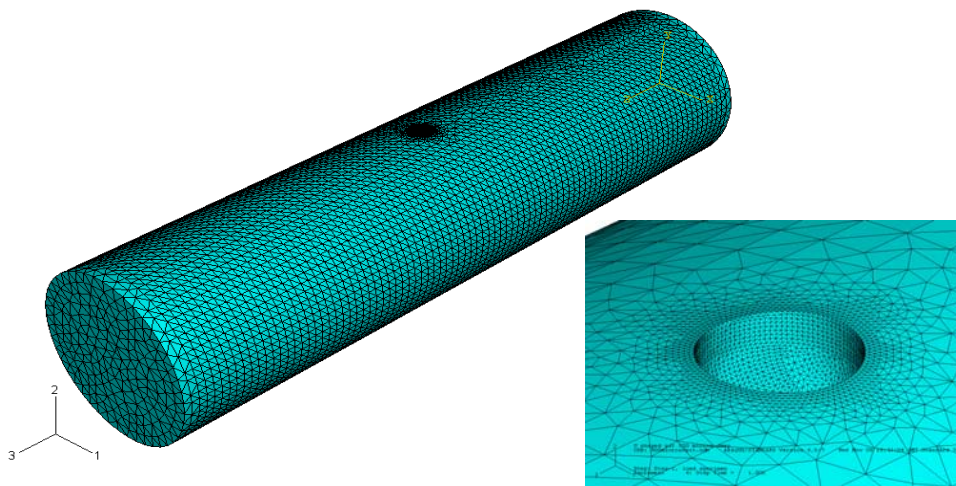
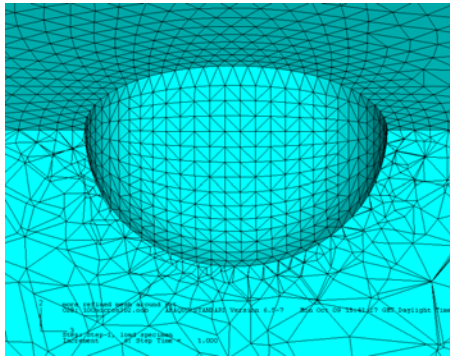
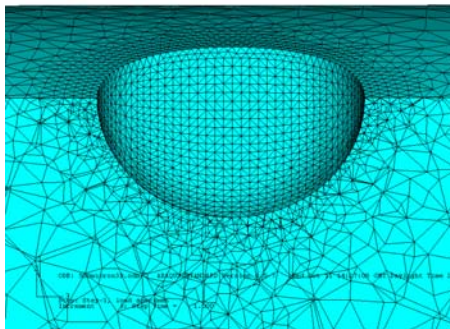


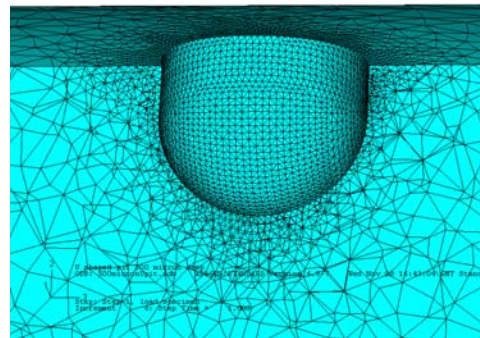
Figure 4. Specimen geometry with mesh structure around 100 μm pit highlighted. Specimen is axially loaded.



100 µm hemi-spherical pit



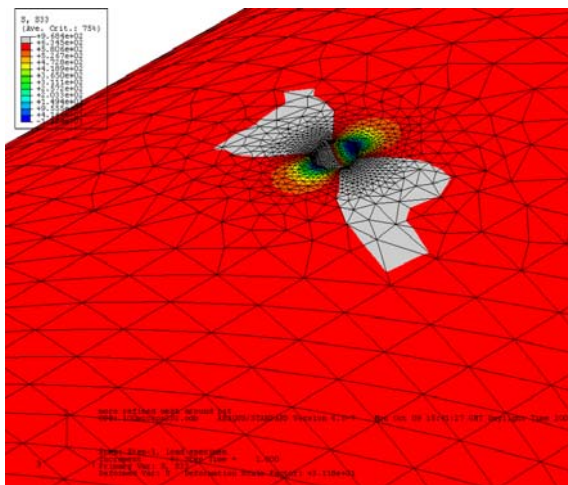
500 µm hemi-spherical pit



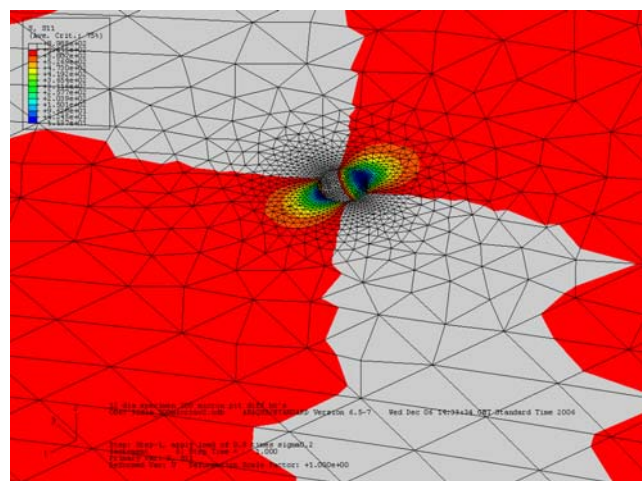
500 µm bullet-shaped pit

Figure 5. Pit geometries showing meshing for different size and type of pit

Figure 6 shows contour plots of axial stress for specimens with a 100 micron pit, and diameters of 6.4 mm and 32 mm respectively. The limits of the contour plots have been adjusted so that the peak of the red contour is set to the applied stress (634.5 MPa).



100 µm pit, 6.4mm dia.



100 µm pit, 32mm dia.

Figure 6. Contour plots of axial stress for specimens with two different diameters: 6.4 mm and 32 mm. Unfortunately, the numbering of the axes for the two diameters is inconsistent but does not affect the results in any way.

These contour plots confirm that the overall stress in both specimens is equivalent to the applied stress. There are some differences in fine detail in these contour plots with an apparent lack of symmetry in stress with distance from the pit but this reflects simply the relatively low values of stress remote from the pit and the nature of the meshing.

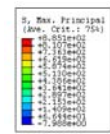
5. RESULTS

A simple representation of the results, taking account of the symmetry of the assumed pit shapes, is to view the data parallel to the stress axis (cut along length) or in cross-section. The results will be presented in this format initially for pits in the 6.4 mm diameter specimen and then for the large, 32 mm diameter, specimen, and finally for the bullet-shaped pit.

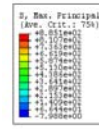
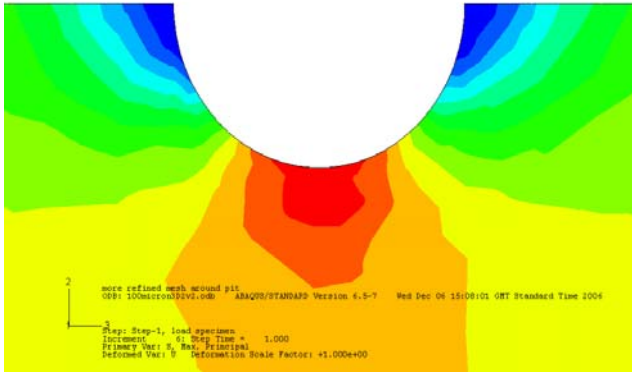
Small diameter (6.4 mm) specimen

The results for a 100 μm hemi-spherical pit are shown in Figure 7. The principal stresses and strains are evaluated in the three dimensions but only the maximum values are quoted. The “maximum principal stress, view cut along length” would represent the axial stress in this case. As might be expected, the stress peaks at the base of the pit when viewed parallel to the stress axis and is quite uniform around the pit when viewed in section, with a decrease towards the pit mouth.

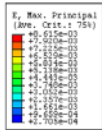
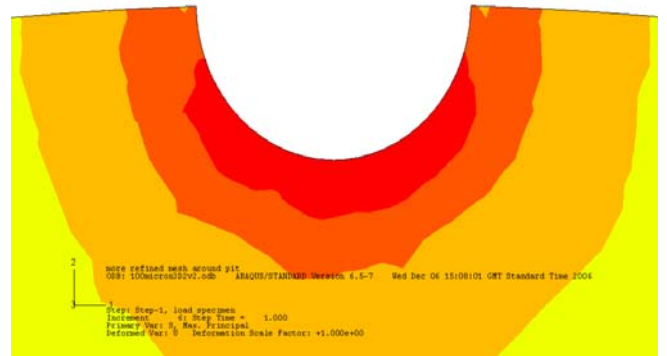
100 μm pit



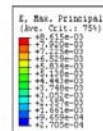
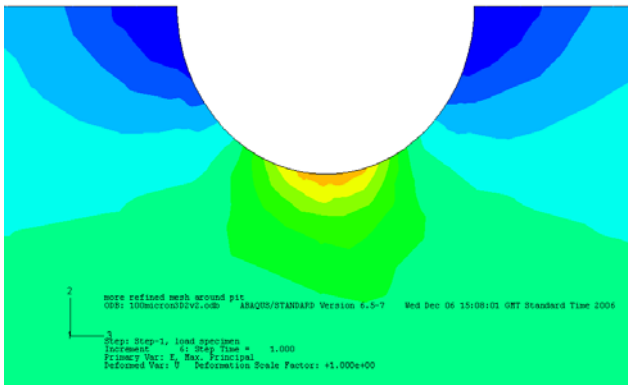
Maximum principal stress,
view cut along length



Maximum principal stress,
cross-section view cut



Maximum principal strain, view
cut along length



Maximum principal strain,
cross-section view cut

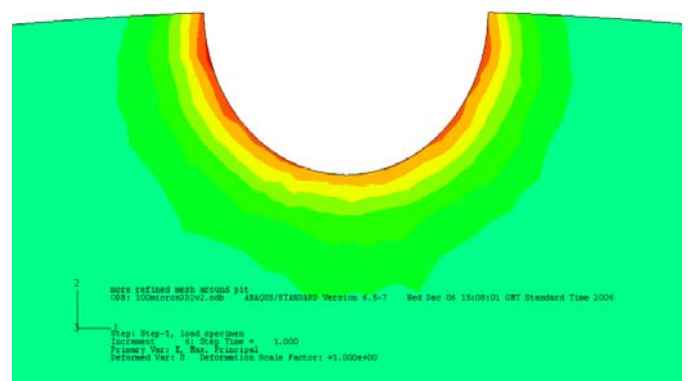


Figure 7. Stress and strain distribution for a 100 μm pit in 6.4 mm diameter specimen.

The surprising feature perhaps is the localisation of strain when viewed in section with the strain attaining a maximum not at the base but just on the pit wall below the pit mouth. This is shown more clearly in Figure 8.

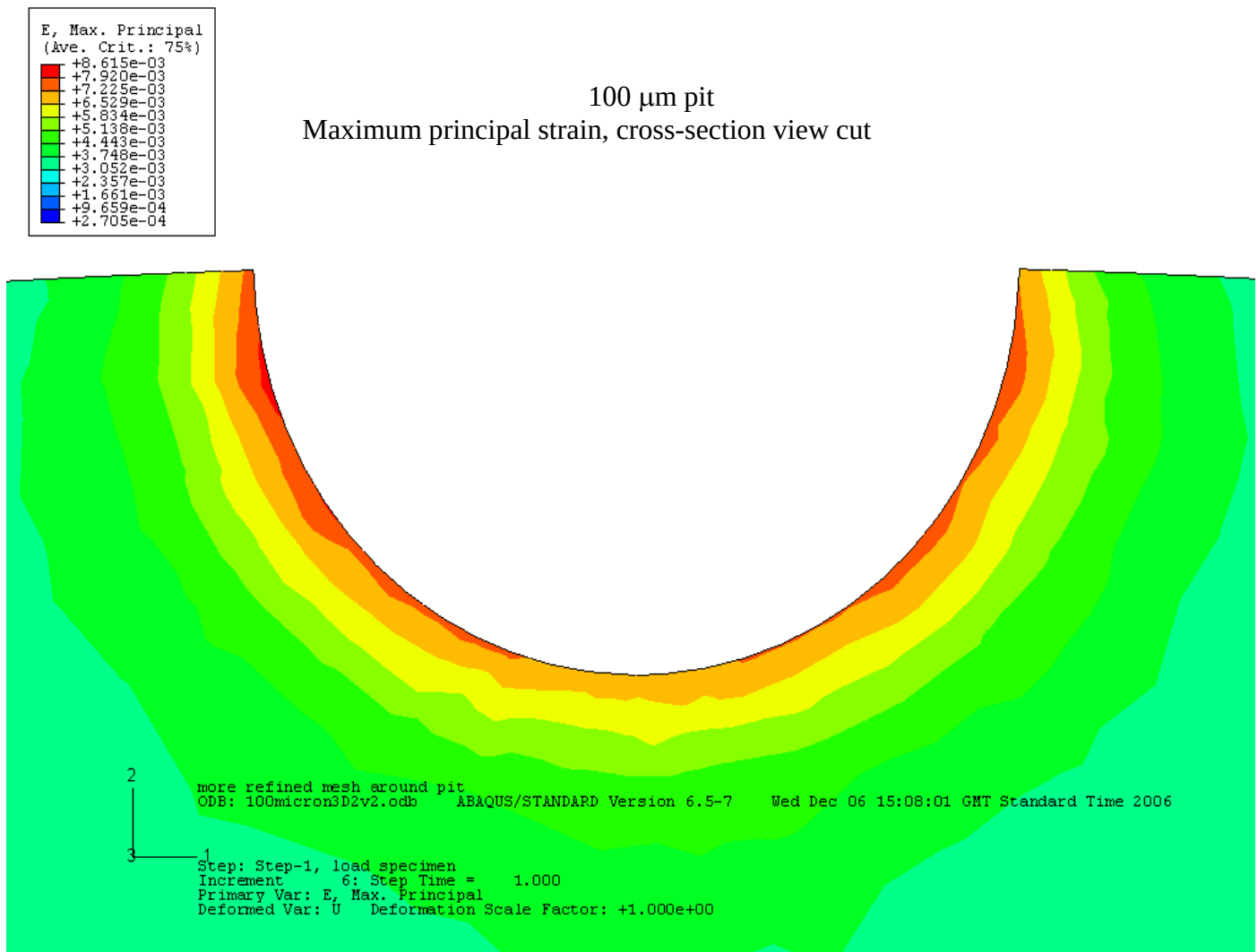
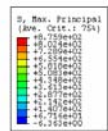


Figure 8. Magnified image of the strain around the 100 μm pit in 6.4 mm diameter when viewed in section showing localisation of strain on the pit wall below the mouth.

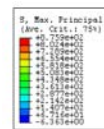
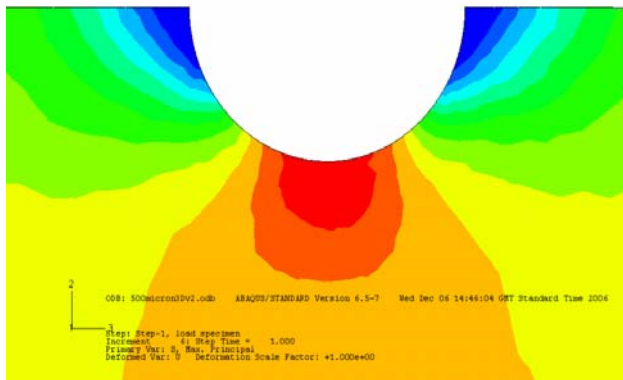
The peak maximum principal strain would lie between 7.9×10^{-3} and 8.6×10^{-3} , above the proportional limit for this steel, indicating localised plastic deformation. The peak maximum principal stress for the 100 μm pit was between 810 MPa and 885 MPa (cf $\sigma_{0.2}$ of 705 MPa). For an ideally smooth pit, as assumed in this model, the strain and stress distribution should not show local fluctuations as would seem to be the case in Figure 8 for example. Such local fluctuations, shown here and later figures, arise from the local meshing and are not real.

The trend in results is replicated for the 500 μm pit as shown in Figures 9 and 10, though with perhaps higher strains at the pit base than observed for the 100 μm pit. Here the peak maximum principal strain was between 8.8×10^{-3} and 9.6×10^{-3} and the peak maximum principal stress between 802 MPa and 876 MPa.

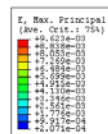
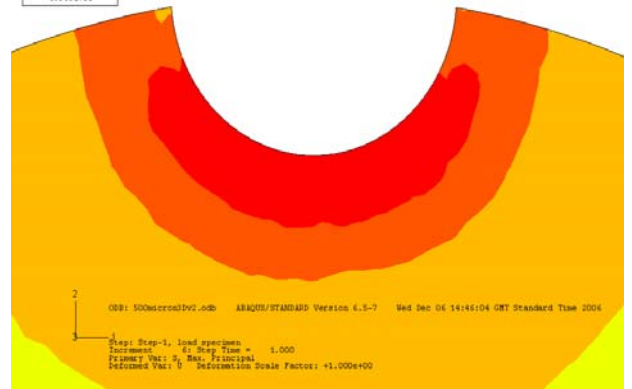
500 μm pit



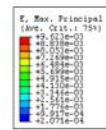
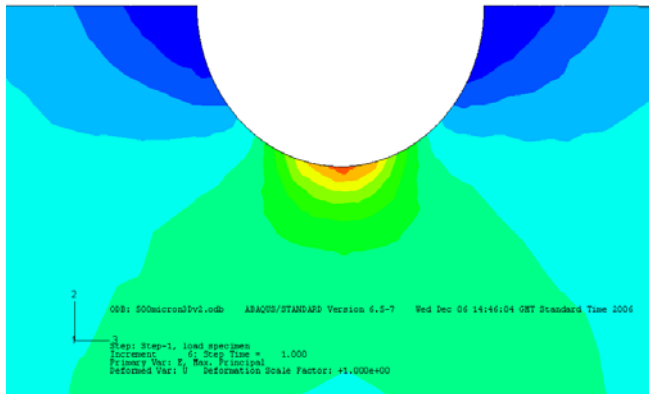
Maximum principal stress,
view cut along length



Maximum principal stress,
cross-section view cut



Maximum principal strain, view cut
along length



Maximum principal strain,
cross-section view cut

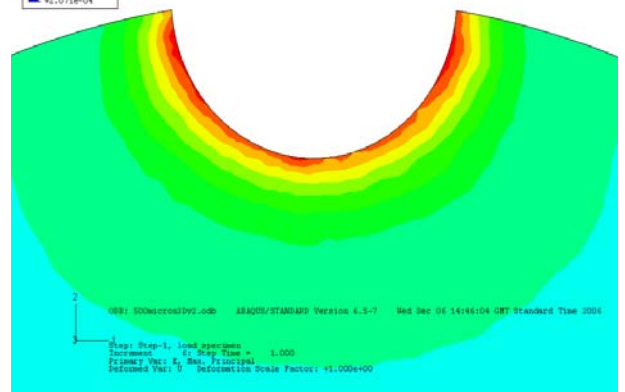


Figure 9. Stress and strain distribution for a 500 μm pit in a 6.4 mm diameter specimen.

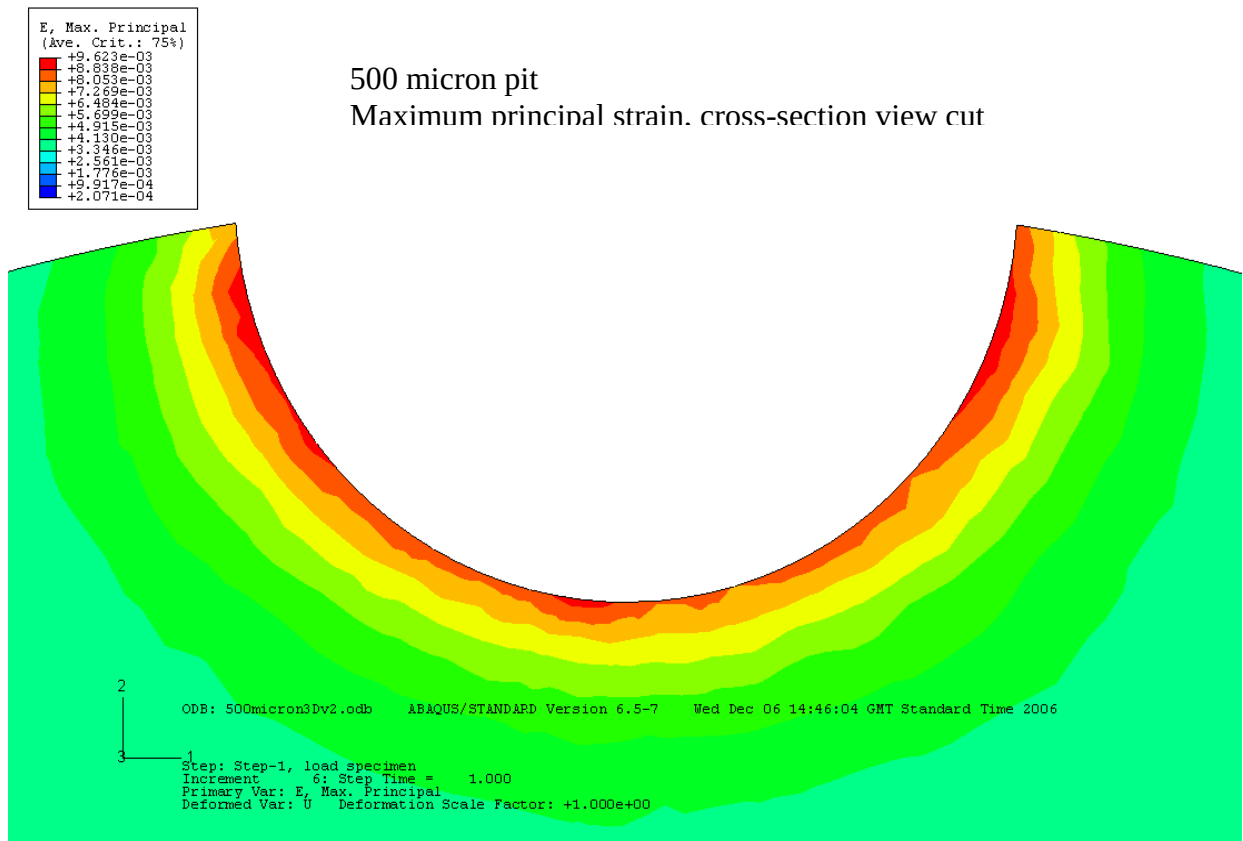


Figure 10. Magnified image of the maximum principal strain around the 500 μm pit in a 6.4 mm diameter specimen when viewed in section showing localisation of strain on the pit wall below the mouth.

Large diameter (32 mm) specimen

The meshing for the larger specimen is shown in Figure 11. To enable comparison of predicted stress and strain values between the different diameter specimens, similar levels of mesh refinement is needed around the pits in both cases. When a consistent level of mesh refinement was applied to the larger diameter specimen the resulting mesh contained many elements, which led to memory problems when running the analysis. To overcome this, the geometry was partitioned, enabling a fine mesh to be created on a smaller region of the geometry and a coarser mesh on the remaining geometry.

100 μm pit, 32 mm diameter specimen

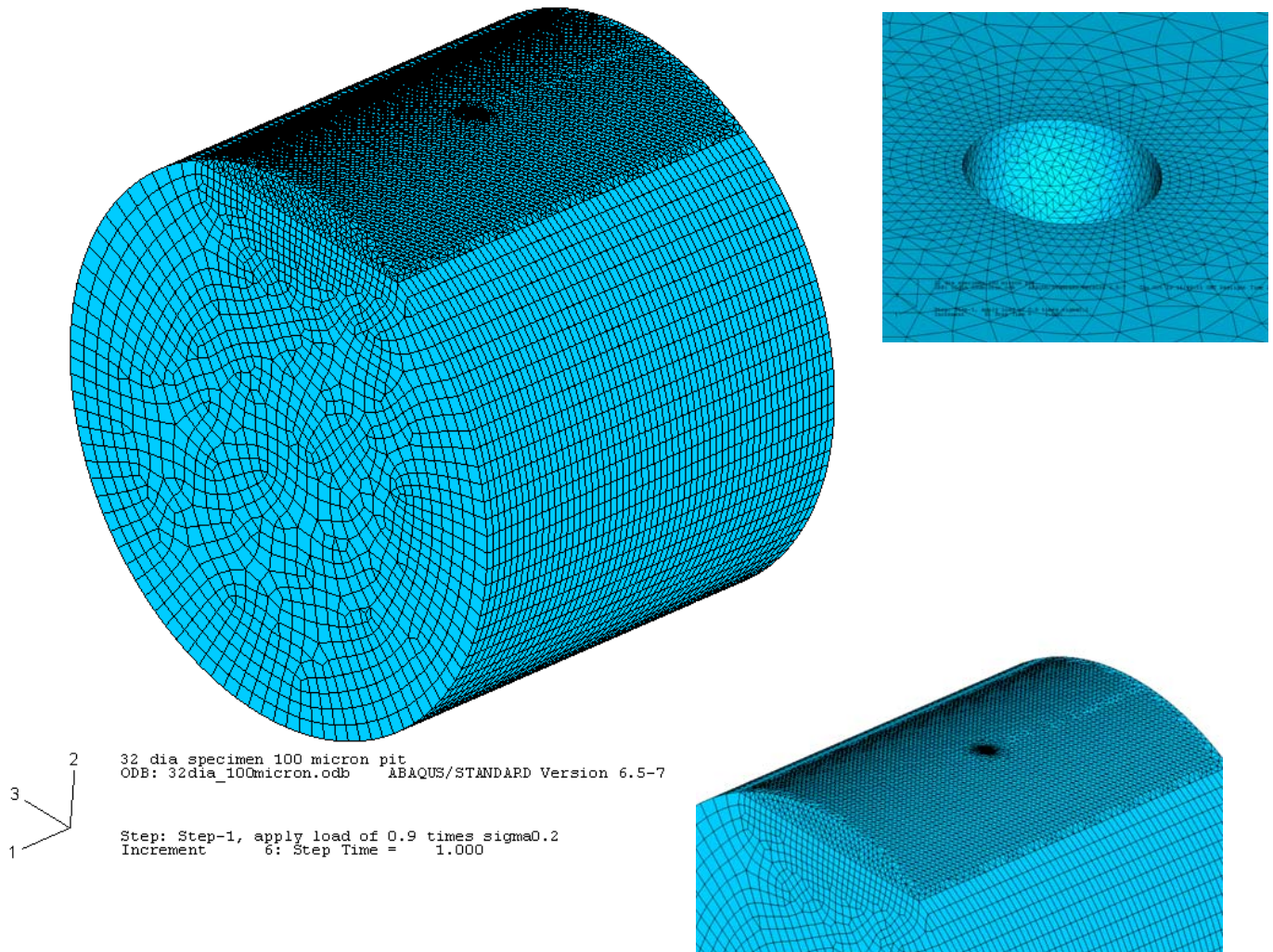
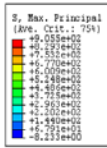


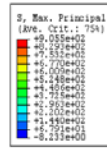
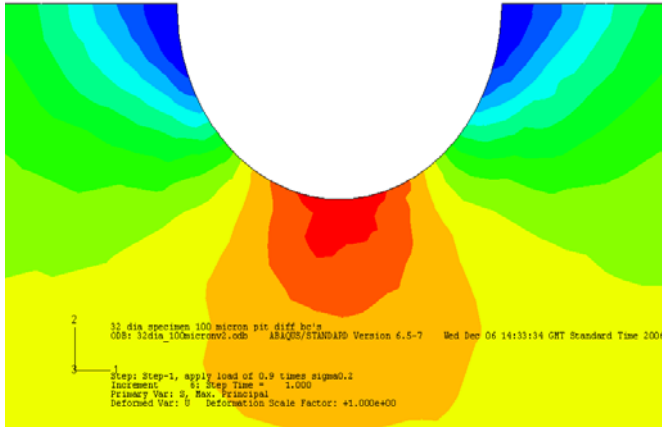
Figure 11. Meshing for 32 mm diameter specimen with 100 μm pit.

The corresponding stress and strain distribution for the 100 μm pit with this size specimen are shown in Figures 12 and 13. The peak maximum principal strain, between 8.0×10^{-3} and 8.7×10^{-3} , is similar to that for the smaller diameter specimen (7.9 - 8.6×10^{-3}) with a similar distribution of strain round the pit. The typical peak maximum principal stress value is similar, between 830 MPa and 900 MPa compared to between 810 MPa and 885 MPa for the 6.4 mm diameter specimens.

100 micron pit, 32 mm diameter



Maximum principal stress, view cut
along length



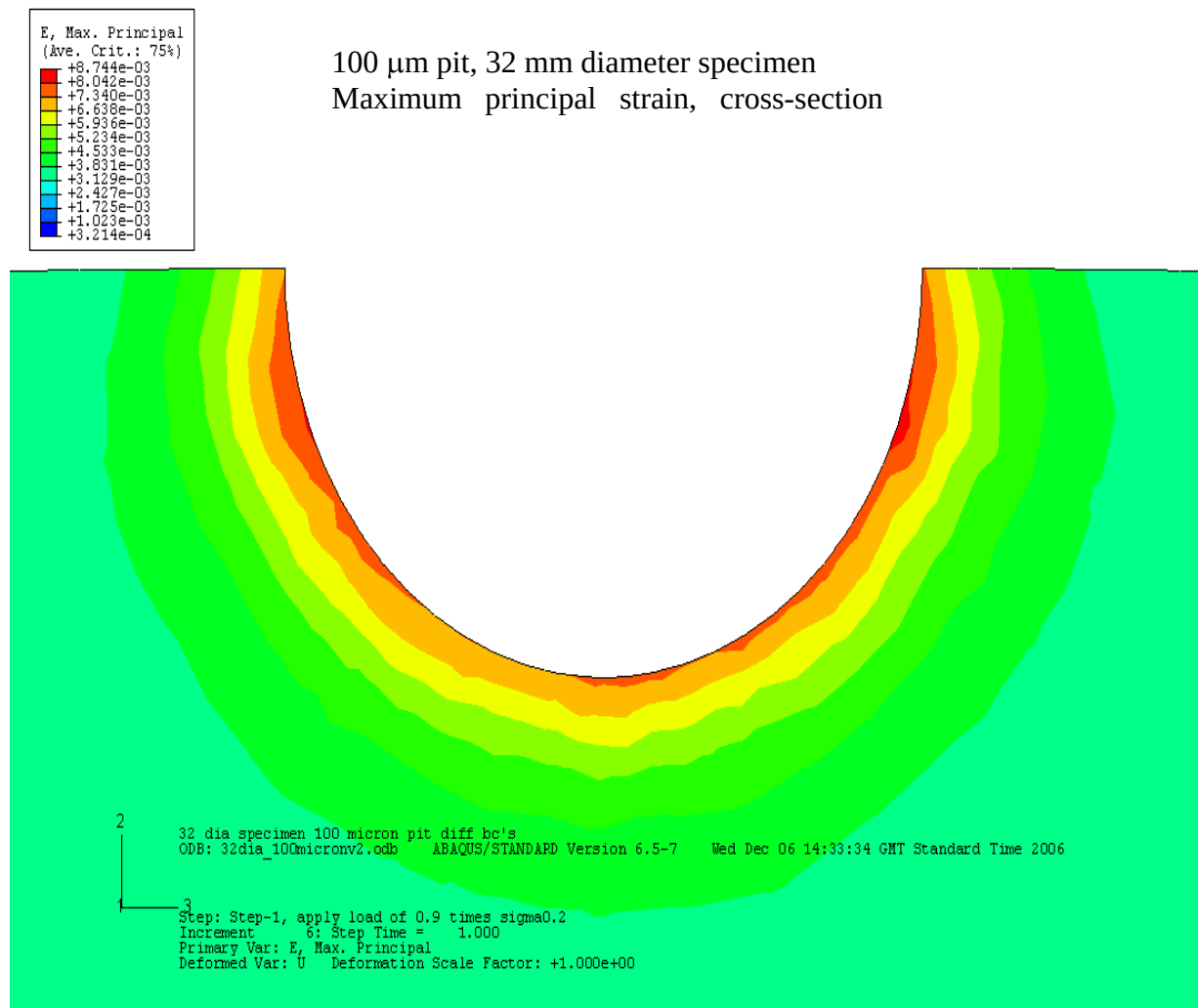
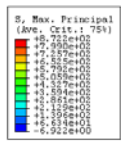


Figure 13. Magnified image of the strain around the 100 μm pit in a 32 mm diameter specimen when viewed in section showing localisation of strain on the pit wall below the mouth.

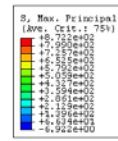
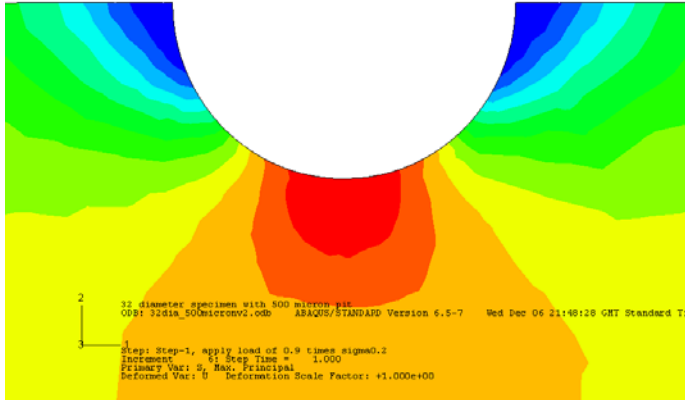
The results for the 500 μm pit in the 32 mm diameter specimen are shown in Figures 14 and 15. The peak maximum principal stress value is between 799 MPa and 870 MPa, similar to that for the smaller diameter specimen. The maximum principal strain distribution is broadly similar to that for the smaller diameter specimen but the peak values, between 8.1×10^{-3} and 8.8×10^{-3} are slightly smaller than calculated for the 6.4 mm diameter specimen, between 8.8×10^{-3} and 9.6×10^{-3} .

Thus, there would appear to be only a very modest effect of the specimen diameter on the strain distribution, confined as expected to the 500 μm pit.

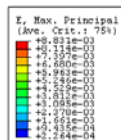
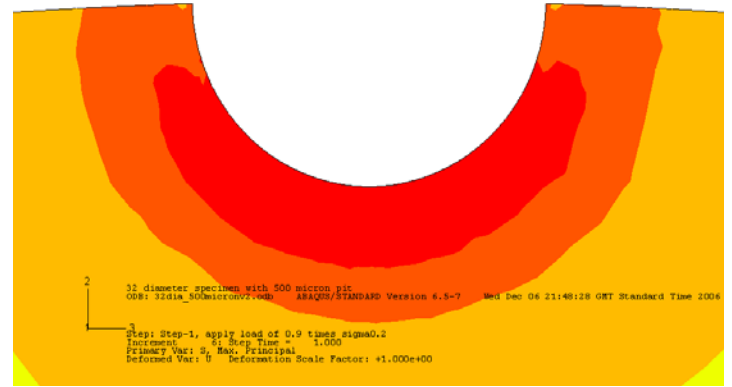
500 μm pit, 32 mm diameter



Maximum principal stress, view cut
along length



Maximum principal stress, cross-
section view cut



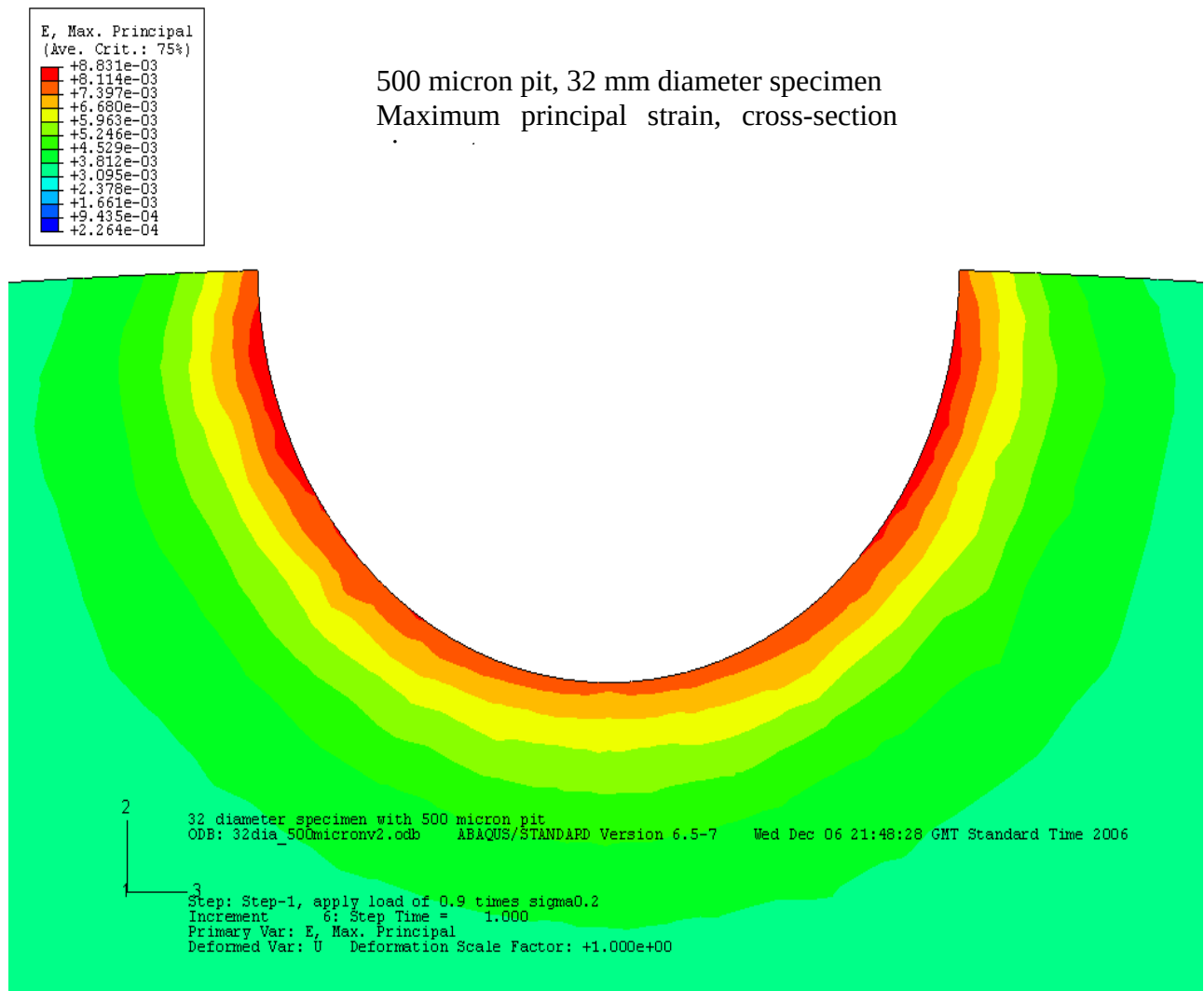
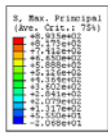


Figure 15. Magnified image of the strain around the 500 μm pit in the 32 mm diameter specimen when viewed in section, showing localisation of strain on the pit wall below the mouth.

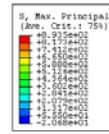
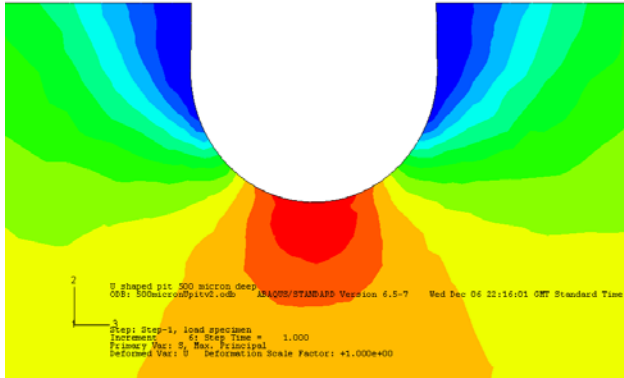
Bullet (U-shaped) pit in small diameter specimen

The stress and strain distribution round a 500 μm pit bullet-shaped pit was examined assuming a 6.4 mm diameter specimen only. This pit shape resembles better the shape of the deeper pits observed experimentally, within the limits of simplified representation. The results are shown in Figures 16 and 17. In broad terms, the trends are similar to that for the hemi-spherical pit, but with more localisation of strain towards the pit mouth. The magnitude of the maximum principal strain is also greater with a peak between 1.1×10^{-3} and 1.2×10^{-2} (cf $8.8\text{--}9.6 \times 10^{-3}$) but the peak in maximum principal stress was similar, between 817 MPa and 893 MPa compared with between 802 MPa and 876 MPa.

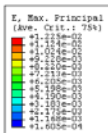
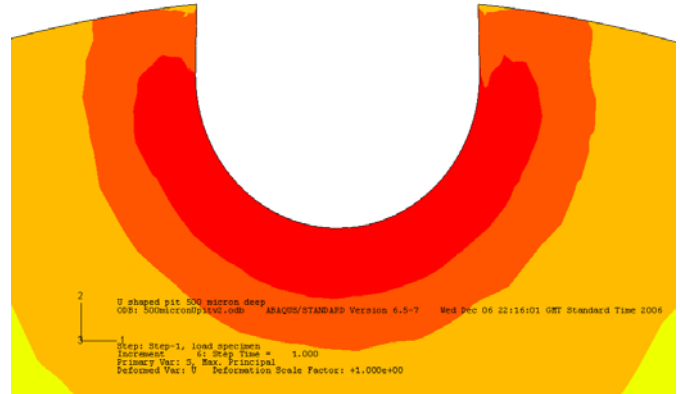
500 μm U-shaped pit



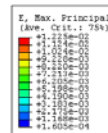
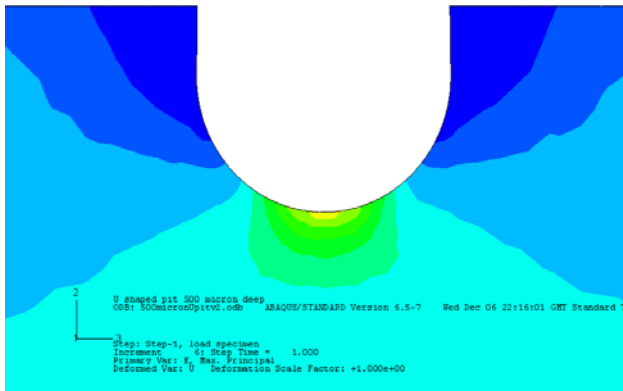
Maximum principal stress, view cut along length



Maximum principal stress, cross-section



Maximum principal strain, view cut along length



Maximum principal strain, cross-section

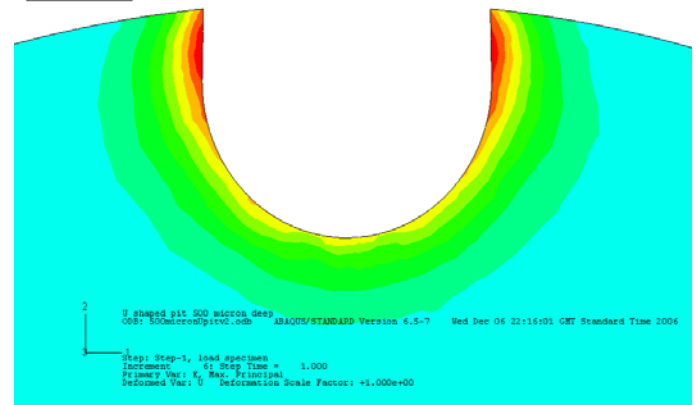


Figure 16. Stress and strain distribution for a 500 μm deep pit in a 6.4 mm diameter specimen.

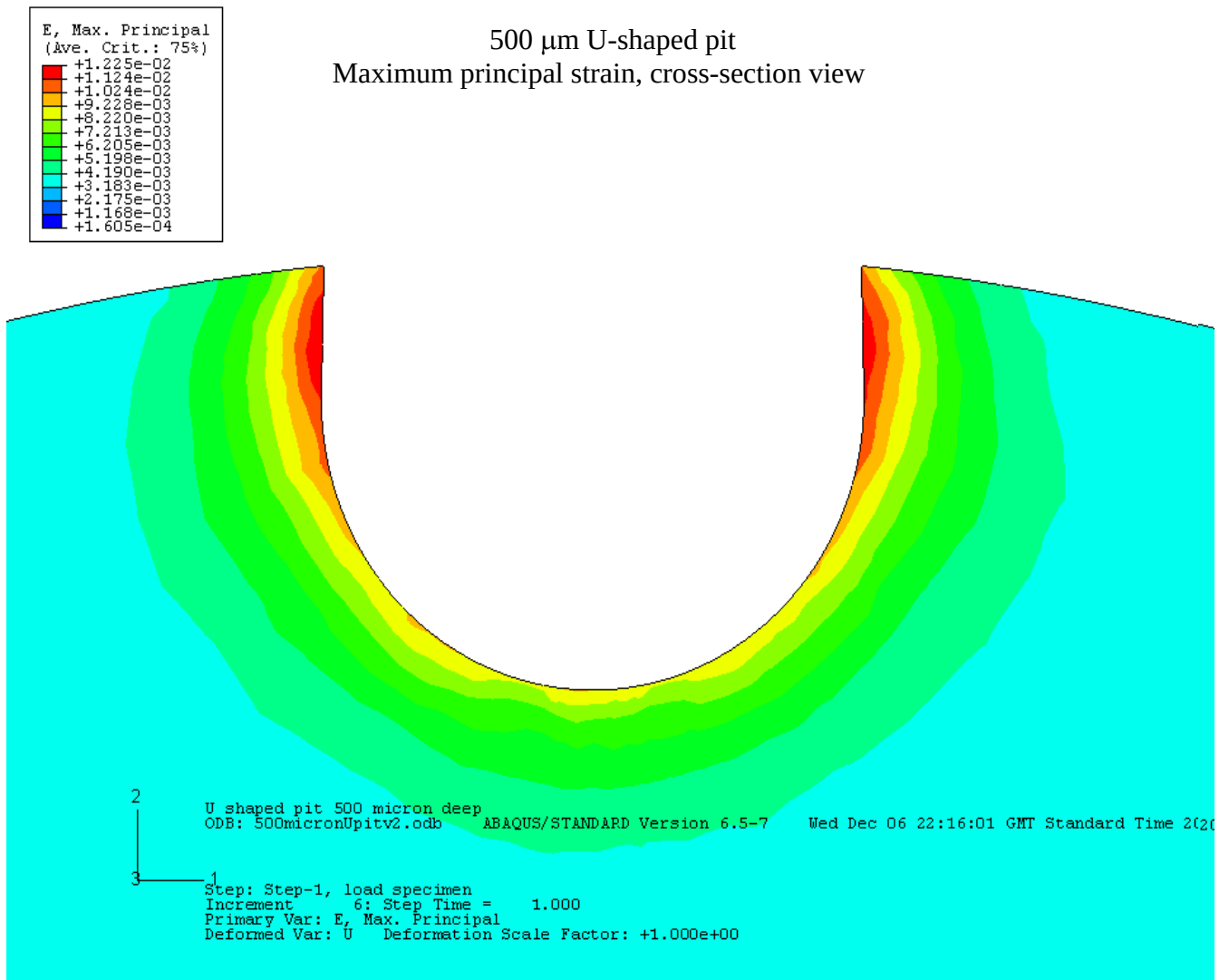


Figure 17. Magnified image of the maximum principal strain around the 500 μm pit in the 6.4 mm diameter specimen when viewed in section, showing localisation of strain on the pit wall just below the mouth.

6. DISCUSSION

The most significant observation from this analysis of relevance to the quest of finding a mechanics-based explanation for the location of crack nucleation from pits is the localisation of plastic strain below the mouth of the pit rather than at the pit base. This is accentuated in the bullet-shaped pit.

In contrast to the distribution of strain, the stress is distributed more uniformly round the pit but decaying towards the pit mouth. This localisation of strain towards the pit mouth, rather than in the highest stress region, reflects a reduced constraint to plastic flow at that location. The usual expectation that the maximum strain will be associated with the maximum stress is linked implicitly to the assumption of elastic strain, which must reflect the stress distribution. However, the ability of the material to deform

plastically depends on other factors and the material will yield where it is energetically most favourable, where there is minimum constraint.

The stress and strain associated with the 500 μm pit for the same applied load was not much different from that of the shallow pit, but with slightly greater strain and to a lesser extent stress. The small difference in stress is not surprising in view of the limited work-hardening of this steel (Figure 3); the steel simply deforms more but with only a modest increase in stress. However, in view of the evolution of the aspect ratio with increasing pit size, direct comparison is more for illustrative purposes and a bullet-shaped pit may be more representative of a deep pit. A key feature to note is the increased localisation of plastic strain on the walls of the bullet-shaped pit near the mouth.

The transition from a pit to a crack depends on exceeding some threshold strain criterion for initiation as well as having a crack growth rate that is greater than the pit growth rate. Feeding into these criteria must also be the distribution of local chemistry and electrode potential within the pit as well as corrosion products. In addition, discrete microstructural/microchemical features such as MnS inclusions may induce local dissolution in a pit, accentuating stress/strain concentration, or may directly favour crack initiation and propagation locally. An added complexity is the absence of direct observation of the nucleation of cracks from pits, as the overall process is too slow for in-situ X-ray tomographical observation, although Figure 2b shows apparently early stages of crack development. Hence, information about the prior history of the pit and crack is inferred from snapshots at different times and potentially this could be misleading. Our understanding is far from complete. Hence, a simple analysis of stress and strain is not going to be sufficient in itself to rationalise all physical observations but provides a piece of information that adds clarity and constraint to possible speculation.

Nucleation of stress corrosion cracks generally results from localised plastic flow, although, depending on the crack growth mechanism, sustained propagation can be affected also directly by the local crack-tip stress distribution. A growing corrosion pit will essentially be inducing a corresponding increase in stress and strain and might be perceived in some respects as inducing a dynamic strain component with a rate associated with the growth rate of the pit. On the basis of this finite element analysis for an ideally smooth and uniform pit surface, and assuming crack nucleation in the region of highest plastic strain, crack emanation from the pit walls might be expected to dominate. Certainly, the results add credence to the perspective derived from extended X-ray tomography studies⁴ that crack initiation appears to occur predominantly, but not exclusively, on the crack walls. There are clear examples of cracks initiating from the pit base but comparatively few. However, whilst localised straining producing bare metal surface is clearly important, the kinetics of reactions on that surface will depend on the local chemistry and potential and variations in within the pit could play a role.

7. CONCLUSIONS

Finite element analysis of the stress and strain distribution around a single pit in a stressed cylindrical specimen has shown that the plastic strain is localised on the pit walls below the pit mouth rather than at the pit base. Reduced constraint to plastic flow is considered to explain the location of extended deformation

This localisation of strain towards the pit mouth is accentuated for bullet-shaped pits, considered more representative of deep pits.

The results suggest localised plastic strain as a contributing factor to the location of crack nucleation from a pit but other variables, including local chemistry and potential within the pit, are additional factors that should not be neglected.

8. REFERENCES

1. A. Turnbull and S. Zhou., Corros. Engng. Sci. Tech., 38, 177-191, 2003.
2. A. Turnbull, S. Zhou and N. McCormick, Corrosion, 62, 555-558, 2006.
3. A. Turnbull, L.N. McCartney and S. Zhou, Scripta Materialia, 54, 575-578, 2006.
4. B. J. Connolly, A Horner, S. Zhou and A. Turnbull, Work in progress.